

Bhattacharyya inequality for quantum state estimation

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Abstract

Using higher-order derivative with respect to the parameter, we will give lower bounds for variance of unbiased estimators in quantum estimation problems. This is a quantum version of the Bhattacharyya inequality in the classical statistical estimation. Because of non-commutativity of operator multiplication, we obtain three different types of lower bounds; Type S, Type R and Type L. If the parameter is a real number, the Type S bound is useful. If the parameter is complex, the Type R and L bounds are useful. As an application, we will consider estimation of polynomials of the complex amplitude of the quantum Gaussian state. For the case where the amplitude lies in the real axis, a uniformly optimum estimator for the square of the amplitude will be derived using the Type S bound. It will be shown that there is no unbiased estimator uniformly optimum as a polynomial of annihilation and/or creation operators for the cube of the amplitude. For the case where the amplitude does not necessarily lie in the real axis, uniformly optimum estimators for holomorphic, antiholomorphic and real-valued polynomials of the amplitude will be derived. Those estimators for the holomorphic and real-valued cases attain the Type R bound, and those for the antiholomorphic and real-valued cases attain the Type L bound. This article clarifies what is the best method to measure energy of laser.

1 Introduction

Quantum estimation is an important theory in quantum information [7, 10]. It is not merely useful for many purposes, for example, evaluation of realized quantum information processing, but also is a fundamental problem in its own right. In this theory, we consider an optimization problem of measurements estimating unknown state, with respect to a risk function under appropriate restriction. A typical case, we adopt in this article, is minimization of variance under unbiasedness condition. What physicists call an observable is an unbiased estimator, and the variance is equal to the mean square error if the estimator is unbiased.

It has been known that the quantum Cramér-Rao inequality gives a lower bound based on first-order derivative and the Schwartz's inequality [7, 10, 18]. Although there is only one Cramér-Rao inequality for classical statistical estimation [12], there are several different inequalities due to the non-commutativity of operator multiplication; SLD-type, RLD-type and LLD-type inequalities formulated by operators respectively called

Symmetric Logarithmic Derivative, Right Logarithmic Derivative and Left Logarithmic Derivative [11]. Yuen and Lax [18] showed that, for the quantum Gaussian state model, the homodyne and heterodyne measurement, respectively, uniformly attains the SLD-type bound for the one-parameter model and the RLD-type bound for the two-parameter model. Nagaoka [14] showed that the SLD bound can be locally attained for all one-parameter models. For asymptotic settings, there are many arguments on the quantum Cramér-Rao bound [1, 5].

For the classical estimation problems, Bhattacharyya [2] has improved the Cramér-Rao inequality extending the order of the derivative. For the classical Gaussian distribution model with unknown mean parameter θ , the uniformly optimum estimator for any polynomial $g(\theta)$ is made by the Hermite polynomials, and it attains the classical Bhattacharyya bound. See [15, 16] for details in classical cases. In the quantum estimation theory, Brody and Hughston [3, 4] defined a Bhattacharyya-type lower bound generalizing the SLD for pure states, and they analyzed asymptotic property.

In this article, first, we will propose three quantum Bhattacharyya inequalities for mixed quantum states with one real or complex parameter. Generalization of the SLD gives the Type S lower bound for the real parameter case, and generalization of RLD and LLD gives the Type R and Type L bounds for the complex parameter case. Second, as the application, we will consider the quantum Gaussian state model where the amplitude parameter θ is unknown. If θ lies in the real axis, the uniformly optimum estimator for θ^2 attaining the Type S bound is a self-adjoint observable given as a superposition of the number counting operator and the homodyne operator. This is realized by squeezing followed by the number counting. For θ^3 , there is no uniformly optimum unbiased estimator written as a polynomial of the creation and/or annihilation operators. If θ lies in the complex plain, we will present uniformly optimum operators for polynomials $g(\theta)$ of θ and $\bar{\theta}$ (the conjugate). If $g(\theta)$ is holomorphic, i.e., $dg/d\bar{\theta} = 0$, then the optimum estimator is given by the heterodyne measurement and it attains the Type R bound. If $g(\theta)$ is anti-holomorphic, i.e., $dg/d\theta = 0$, then the optimum estimator is also given by the heterodyne measurement and it attains the Type L bound. If $g(\theta)$ is real-valued, i.e., $g(\theta) = \overline{g(\theta)}$, the optimum estimator is given by some polynomials of the annihilation/creation operators and it attains both Type R and Type L bounds.

In quantum optics, the Gaussian state is a simple model of laser whose complex amplitude is fluctuated around $\theta \in \mathbb{C}$, and the energy of the laser is proportional to $|\theta|^2$. Using the Type R and L inequality, we will see that the counting measurement is optimum. If $\theta \in \mathbb{R}$ is previously known, the Type S inequality shows that a counting measurement after a squeezing operation is optimum.

This article is constructed as follows. In Section 2, our problem will be formulated and a known proposition of the quantum Cramér-Rao inequality will be shown. In Section 3, new theoretical results of quantum Bhattacharyya inequality will be presented. In Section 4, our theory will be applied to the quantum Gaussian state model. Appendix A is the proof for Section 3, and Appendix B is that for Section 4.

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2 Setup

Suppose that there is a quantum system with an unknown state. Consider a set of candidate states $\{\rho_\theta\}$ for the system parameterized by $\theta \in \Theta$. In this article, it is assumed that these density operators are invertible and that $\Theta = \mathbb{R}$ or $\Theta = \mathbb{C}$. We will use ζ as the parameter instead of θ when we need to remark that the parameter may not be a real number. Our interest is to estimate the true value of $g(\theta)$, where $g : \Theta \rightarrow \Theta$ is a smooth function. Since the probabilistic error is inevitable, we consider an optimization problem of estimation under some restriction.

An estimator M for $g(\theta)$ is a Positive Operator Valued Measure (POVM) taking measurement outcomes in Θ . (In a strict definition, an estimator should take measurement outcomes in $g(\Theta) \supseteq \Theta$, but, for theoretical convenience, we adopt the weaker definition in this article.)

The expectation (=average=mean) of M is

$$E[M] := \int_{\omega \in \Theta} \omega \text{Tr}[\rho_\theta M(d\omega)].$$

If $E[M] = g(\theta)$ for any $\theta \in \Theta$, M is said to be unbiased. We adopt the variance of M as the risk function; the variance is defined, in this article, as

$$\begin{aligned} V[M] &:= \int_{\omega \in \Theta} |\omega - E[M]|^2 \text{Tr}[\rho_\theta M(d\omega)] \\ &= \int_{\omega \in \Theta} (\omega - E[M]) \overline{(\omega - E[M])} \text{Tr}[\rho_\theta M(d\omega)]. \end{aligned}$$

An unbiased estimator with the minimum variance among all unbiased estimators at a point $\theta \in \Theta$ is said to be locally optimum at θ . If an unbiased estimator is optimum at any $\theta \in \Theta$, it is said to be uniformly optimum.

The lower bound for the variance of unbiased estimators has been given by using the Schwartz's inequality and the first-order derivative with respect to θ . This bound is called the quantum Cramér-Rao inequality. See [7, 8, 9, 10, 11, 18] for the proof and related topics.

Proposition *Assume that $\Theta = \mathbb{R}$, the variance of any unbiased estimator M for $g(\theta)$ satisfies*

$$V[M] \geq |g'(\theta)|^2 / J^S. \quad (1)$$

If $T := g'(\theta)(J^S)^{-1}L^S + g(\theta)$ (A scalar x is identified with x times identity.) is free of the parameter, then the Projection Valued Measure (PVM) taking measurement outcomes in \mathbb{R} given by the self-adjoint operator T is the uniformly optimum unbiased estimator for $g(\theta)$ and the equality holds for (1).

Assume that $\Theta = \mathbb{C}$, the variance of any unbiased estimator M for $g(\zeta)$ ($\zeta \in \Theta$) satisfies

$$V[M] \geq |g'(\zeta)|^2 / J^R, \quad (2)$$

$$V[M] \geq |g'(\bar{\zeta})|^2 / J^L. \quad (3)$$

If $T := g'(\zeta)(J^R)^{-1}L^R + g(\zeta)$ is free of the parameter and if T is normal, i.e., $TT^\dagger = T^\dagger T$, then the PVM taking measurement outcomes in \mathbb{C} given by the spectrum decomposition

of T is the uniformly optimum unbiased estimator for $g(\zeta)$ and the equality holds for (2). Similarly, if $T := \bar{g}'(\bar{\zeta})(J^L)^{-1}L^L + g(\zeta)$ is free of the parameter and is normal, it is the uniformly optimum unbiased estimator and the equality holds for (3).

Here, J^S , L^S , J^R , L^R , J^L and L^L are defined as follows.

Definition of L^S and J^S . For the case $\Theta = \mathbb{R}$, let L^S be a self-adjoint operator satisfying

$$\frac{d}{d\theta}\rho_\theta = \frac{\rho_\theta L^S + L^S \rho_\theta}{2}, \quad (4)$$

and then define J^S as $\text{Tr}[\rho_\theta(L^S)^2]$. L^S is called Symmetric Logarithmic Derivative (SLD) and J^S is called SLD Fisher information.

Definition of L^R , L^L , J^R and J^L . For the case $\Theta = \mathbb{C}$, let L^R and L^L be operators satisfying

$$\frac{d}{d\bar{\zeta}}\rho_\zeta = \rho_\zeta L^R, \quad \frac{d}{d\zeta}\rho_\zeta = L^L \rho_\zeta \quad (5)$$

where $\zeta := x + \sqrt{-1}y$, $d/d\zeta := (d/dx - \sqrt{-1}d/dy)/2$ and $d/d\bar{\zeta} := (d/dx + \sqrt{-1}d/dy)/2$ for real variables x and y . Then J^R and J^L are defined as $\text{Tr}[\rho_\zeta L^R(L^R)^\dagger]$ and $\text{Tr}[L^L \rho_\zeta (L^L)^\dagger]$. L^R is called Right Logarithmic Derivative (RLD) and J^R is called RLD Fisher information. Similarly, L^L is called Left Logarithmic Derivative (LLD) and J^L is LLD Fisher information.

The definitions of L^S , L^R and L^L are not unique because the equations (4) and (5) have many solutions on a space where ρ_θ does not depend on θ . For example, the heterodyne measurement for the Gaussian model is obtained in the form $(J^R)^{-1}L^R + \theta$ ($\theta \in \mathbb{C}$) where L^R is a solution in an extended system with an ancilla state, while the homodyne measurement $(J^S)^{-1}L^S + \theta$ ($\theta \in \mathbb{R}$) needs no extension. In spite of the ambiguity of L , the inner product J is uniquely determined.

When the sample size is finite, there is no unbiased estimators uniformly optimum except for a few cases where the parameter space is flat with respect to the metric defined by J^S [13]. When ρ_θ is not smooth with respect to θ , the difference instead of the derivative is useful [17].

There may be cases where the unbiasedness condition is so strict that no estimator is unbiased, and where the variance (or the means square error) is not appropriate as the risk geometrically. However, it is worth studying such problems with a view to gaining theoretical insight.

3 Quantum Bhattacharyya inequality

The quantum Cramér-Rao inequality is generalized by using higher-order derivative instead of the first-order derivative.

3.1 Quantum Bhattacharyya inequality of Type S for the real parameter case

Consider the case $\Theta = \mathbb{R}$. Let $L_k^S := {}^t(L_1, L_2, \dots, L_k)$ be a column vector of self-adjoint operators satisfying

$$\frac{d^k}{d\theta^k} \rho_\theta = \frac{\rho_\theta L_k + L_k \rho_\theta}{2}. \quad (6)$$

To simplify notations, we introduce a column vector $D_k := {}^t(d/d\theta, \dots, d^k/d\theta^k)$ of differential operators, and we write (6) as

$$D_k[\rho_\theta] = \frac{\rho_\theta L_k^S + L_k^S \rho_\theta}{2}.$$

Let J_k^S be a $k \times k$ matrix where the (i, j) -th entry is

$$J_{i,j} := \text{Tr}[\rho_\theta L_i L_j].$$

The definition of J_k^S is also simplified as $J_k^S = \text{Tr}_{k \times k}[\rho_\theta L_k^S {}^t(L_k^S)]$ where $\text{Tr}_{m \times n}[A]$ means taking the trace of each entry of an $m \times n$ matrix A , namely,

$$\text{Tr}_{m \times n} \left[\begin{pmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & \ddots & \vdots \\ A_{m,1} & \cdots & A_{m,n} \end{pmatrix} \right] = \begin{pmatrix} \text{Tr}[A_{1,1}] & \cdots & \text{Tr}[A_{1,n}] \\ \vdots & \ddots & \vdots \\ \text{Tr}[A_{m,1}] & \cdots & \text{Tr}[A_{m,n}] \end{pmatrix}.$$

Though the definition of L_k^S is not unique for a system extension with a known ancilla state, J_k^S is uniquely determined.

Assume that J_k^S is invertible. The Quantum Bhattacharyya inequality of ‘Type S’ is given as follows.

Theorem 1 *If M is an unbiased estimator for $g(\theta)$, it holds that*

$$V[M] \geq {}^t(D_k[g(\theta)])(J_k^S)^{-1} D_k[g(\theta)]. \quad (7)$$

Epecially, if $T := {}^t D_k[g(\theta)](J_k^S)^{-1} L_k^S + g(\theta)$ is free of the parameter, then the PVM M given by the self-adjoint observable T is the uniformly optimum unbiased estimator and the equality holds for (7).

See Appendix A for the proof.

3.2 Quantum Bhattacharyya inequality of Type R and Type L for the complex parameter case

Consider the case $\Theta = \mathbb{C}$. Let $D_k^{\mathbb{C}}$ be a column vector

$$D_k^{\mathbb{C}} := {}^t \left(\frac{d}{d\zeta}, \frac{d}{d\bar{\zeta}}, \frac{d^2}{d\zeta^2}, \frac{d^2}{d\zeta d\bar{\zeta}}, \frac{d^2}{d\bar{\zeta}^2}, \dots, \frac{d^k}{d\zeta^k}, \dots, \frac{d^k}{d\zeta^{k-l} d\bar{\zeta}^l}, \dots, \frac{d^k}{d\bar{\zeta}^k} \right),$$

where

$$\frac{d^m}{d\zeta^n d\bar{\zeta}^{m-n}} := \frac{1}{2^m} \left(\frac{d}{dx} - \sqrt{-1} \frac{d}{dy} \right)^n \left(\frac{d}{dx} + \sqrt{-1} \frac{d}{dy} \right)^{m-n}.$$

The number of the entries is $K := k(k+3)/2$. Define column vectors L_k^R and L_k^L of K operators as the solutions to the equations

$$D_k^{\mathbb{C}}[\rho_\zeta] = \rho_\zeta L_k^R, \quad D_k^{\mathbb{C}}[\rho_\zeta] = L_k^L \rho_\zeta.$$

Let J_k^R and J_k^L be $K \times K$ matrices given by

$$J_k^R := \text{Tr}_{K \times K}[\rho_\zeta L_k^R (L_k^R)^\dagger], \quad J_k^L := \text{Tr}_{K \times K}[L_k^L \rho_\zeta (L_k^L)^\dagger],$$

where

$$\begin{pmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & \ddots & \vdots \\ A_{m,1} & \cdots & A_{m,n} \end{pmatrix}^\dagger := \begin{pmatrix} A_{1,1}^\dagger & \cdots & A_{m,1}^\dagger \\ \vdots & \ddots & \vdots \\ A_{1,n}^\dagger & \cdots & A_{m,n}^\dagger \end{pmatrix}.$$

Applying this notation to $D_k^{\mathbb{C}}$, we define

$$D_k^{\mathbb{C}\dagger} := \left(\frac{d}{d\bar{\zeta}}, \frac{d}{d\zeta}, \frac{d^2}{d\bar{\zeta}^2}, \frac{d^2}{d\zeta d\bar{\zeta}}, \frac{d^2}{d\zeta^2}, \dots, \frac{d^k}{d\bar{\zeta}^k}, \dots, \frac{d^k}{d\zeta^l d\bar{\zeta}^{k-l}}, \dots, \frac{d^k}{d\zeta^k} \right).$$

The definitions of L_k^R and L_k^L are not unique due to the system extension with a known ancilla state, but those of J_k^R and J_k^L are unique.

The Quantum Bhattacharyya inequalities of Type R and Type L are given as follows.

Theorem 2 *If M is an unbiased estimator for $g(\zeta)$, then it holds that*

$$V[M] \geq D_k^{\mathbb{C}\dagger}[g(\zeta)](J_k^R)^{-1} D_k^{\mathbb{C}}[g(\bar{\zeta})], \quad (8)$$

$$V[M] \geq D_k^{\mathbb{C}\dagger}[g(\zeta)](J_k^L)^{-1} D_k^{\mathbb{C}}[g(\bar{\zeta})]. \quad (9)$$

Especially, if $T := D_k^{\mathbb{C}\dagger}[g(\zeta)](J_k^R)^{-1} L_k^R + g(\zeta)$ is free of the parameter and if T is normal, then the PVM given by the spectrum decomposition of T is the uniformly optimum unbiased estimator and the equality holds for (8). Similarly, if $T := D_k^{\mathbb{C}\dagger}[g(\zeta)](J_k^L)^{-1} L_k^L + g(\zeta)$ is free of the parameter, it is the uniformly optimum unbiased estimator and the equality holds for (9).

See Appendix A for the proof.

4 Application to the quantum Gaussian model

For a known constant $N > 0$ and an unknown parameter $\theta \in \Theta$, let

$$\rho_\theta := \frac{1}{\pi N} \int_{\alpha \in \mathbb{C}} \exp\left(-\frac{|\alpha - \theta|^2}{N}\right) |\alpha\rangle \langle \alpha| d^2 \alpha.$$

Here, $d^2 \alpha$ means $dx dy$ where $\alpha = x + \sqrt{-1}y$, and $|\alpha\rangle$ is the coherent vector of the complex amplitude $\alpha := x + \sqrt{-1}y$, i.e.,

$$|\alpha\rangle := \exp\left(-\frac{|\alpha|^2}{2}\right) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e_n$$

where $\{e_n\}_{n=0}^\infty$ is the orthonormal system.

The quantum Gaussian model is a generalization of the classical model of Gaussian distributions, where the probability density is given as

$$f_\theta(x) := \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x-\theta)^2}{2}\right).$$

Here, $\theta \in \mathbb{R}$ is unknown. In the classical estimation problem of θ^k , the k -th Hermite polynomial $T(x) := (-1)^k e^{x^2/2} (d^k/dx^k) e^{-x^2/2}$ is the uniformly optimum unbiased estimator which attains the classical Bhattacharyya lower bound.

For the quantum Gaussian model, we consider two models; the real Gaussian model $\Theta = \mathbb{R}$ and the complex Gaussian model $\Theta = \mathbb{C}$. For the real Gaussian model, we consider two cases; $g(\theta) = \theta^2$ and $g(\theta) = \theta^3$. For $g(\theta) = \theta^2$, the optimum estimator is given by a PVM with measurement outcomes in $\Theta (= \mathbb{R} \supsetneq g(\Theta) = \{x \mid x \geq 0\})$. For $g(\theta) = \theta^3$, it will be shown that any unbiased estimator given by an observable as a polynomial of the creation/annihilation operators can not be uniformly optimum. We will identify a self-adjoint operator with the PVM.

Theorem 3 *Suppose that $\Theta = \mathbb{R}$.*

If $g(\theta) = \theta^2$, then the unbiased estimator

$$T = \frac{N(N+1)}{(2N+1)^2} (a^2 + a^{\dagger 2}) + \frac{N^2 + (N+1)^2}{(2N+1)^2} a^\dagger a - N \frac{N^2 + (N+1)^2}{(2N+1)^2} \quad (10)$$

uniformly attains the Type S lower bound, so T is uniformly optimum. Here, a is the annihilation operator satisfying $ae_n = \sqrt{n}e_{n-1}$ and $aa^\dagger - a^\dagger a = I$ (identity).

If $g(\theta) = \theta^3$, no unbiased estimator of the polynomial form of the creation/annihilation operators can be uniformly optimum.

See Appendix B.1 for the proof.

The value $g(\theta) = \theta^2$ may be measured by the counting measurement $a^\dagger a$ -constant, or by the square of the homodyne measurement $(a + a^\dagger)^2$ -constant. This theorem says that the optimum estimator is a superposition of these two measurements. We also note that this optimum estimator is realized as the counting measurement $b^\dagger b$ -constant after the following squeezing operation on the system;

$$\begin{pmatrix} a \\ a^\dagger \end{pmatrix} \mapsto \frac{1}{\sqrt{2N+1}} \begin{pmatrix} N+1 & N \\ N & N+1 \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} =: \begin{pmatrix} b \\ b^\dagger \end{pmatrix}.$$

For the complex Gaussian model, we will consider these three cases for a polynomial $g(\zeta)$ of $\zeta \in \mathbb{C}$;

Holomorphic case: $dg(\zeta)/d\bar{\zeta} \equiv 0$,

Antiholomorphic case: $dg(\zeta)/d\zeta \equiv 0$,

Real-valued case: $g(\zeta) \equiv g(\bar{\zeta})$.

In each case, an optimal unbiased estimator will be presented by a PVM taking measurement outcomes in \mathbb{C} .

A PVM M taking outcomes in \mathbb{C} will be described by a normal operator T , that is, $TT^\dagger = T^\dagger T$ and

$$T = \int_{\omega \in \mathbb{C}} \omega M(d\omega).$$

Since $E[M] = \text{Tr}[\rho T]$, it holds that

$$V[M] = \text{Tr}[\rho_\theta (T - E[T])(T - E[T])^\dagger] = \text{Tr}[\rho_\theta (T - E[T])^\dagger (T - E[T])].$$

See [6] for details on normality and subnormality of operators for quantum measurement.

For the holomorphic and antiholomorphic cases, we need to extend the system to describe the normal operators. Let \mathcal{K} be an ancilla system spanned by $\{f_n\}_{n=0}^\infty$, and let b be the annihilation operator satisfying $bf_n = \sqrt{n}f_{n-1}$ and $bb^\dagger - b^\dagger b = 1$. Namely, the original annihilation operator a means $a \otimes I$, and the new one b may represent $I \otimes a$. The original state ρ_ζ is extended to $\rho_\zeta \otimes f_0 f_0^\dagger$.

Theorem 4 *Suppose that $\Theta = \mathbb{C}$ and $g(\theta)$ is a polynomial of θ and $\bar{\theta}$.*

If $g(\theta)$ is holomorphic, the unbiased estimator

$$T = g(a + b^\dagger)$$

uniformly attains the Type R lower bound, so it is uniformly optimum.

If $g(\theta)$ is antiholomorphic, the unbiased estimator

$$T = \bar{g}(a^\dagger + b)$$

uniformly attains the Type L lower bound so it is uniformly optimum, where $\bar{g}(z) := \overline{g(z)}$.

If $g(\theta)$ is real-valued, the unbiased estimator

$$\begin{aligned} T = & \sum_{m,n} c_{m,n} (N+1)^n \sum_{r=0}^{\min(m,n)} (-1)^{\min(m,n)-r} \binom{\max(m,n)}{\min(m,n)-r} \\ & \times \frac{\min(m,n)!}{r!} \left(\frac{a}{N+1} \right)^{r+\max(0,n-m)} a^{\dagger r+\max(0,m-n)} \end{aligned}$$

uniformly attains both Type R and Type L lower bounds so it is uniformly optimum, where $g(z) = \sum_{m,n} c_{m,n} \theta^m \bar{\theta}^n$.

See Appendix B.2 for the proof.

For the holomorphic and antiholomorphic cases, the optimum estimators are realized essentially by the heterodyne measurement, that is, the estimated values for $g(a + b^\dagger)$ and $\bar{g}(a^\dagger + b)$ are both obtained by operating $g(\cdot)$ to the heterodyne outcome. Hence they can be simultaneously carried out. On the other hand, for the real-valued case, no ancilla system is used so that it can not be measured simultaneously with the holomorphic/antiholomorphic cases.

For a real-valued case $g(\theta) = \text{Re}(\theta)^2$, the optimum estimator is of the form $(a + a^\dagger)^2/4 - \text{constant}$, i.e., the square of the homodyne measurement. This measurement does not commute with that for $g(\theta) = \theta^2$ ($\theta \in \mathbb{R}$) of Theorem 3.

Appendices

The proofs for Theorems 1 and 2 will be given in Appendix A, and those for Theorems 3 and 4 will be given in Appendix B.

A Proofs of Theorems 1 and 2

The first lemma implies that, for any POVM estimator for $g(\theta)$, there is a PVM which has the same expectation and a smaller variance.

Lemma 1 *Assume that M is a POVM taking measurement outcomes in Θ . Let*

$$T = \int_{\omega \in \Theta} \omega M(d\omega).$$

Then, it holds that

$$\int_{\omega \in \Theta} |\omega|^2 \text{Tr}[\rho_\theta M(d\omega)] \geq \text{Tr}[\rho_\theta T T^\dagger], \quad (11)$$

$$\int_{\omega \in \Theta} |\omega|^2 \text{Tr}[\rho_\theta M(d\omega)] \geq \text{Tr}[\rho_\theta T^\dagger T]. \quad (12)$$

Proof. The first formula (11) is obtained by

$$\begin{aligned} & \int_{\omega \in \Theta} |\omega|^2 \text{Tr}[\rho_\theta M(d\omega)] - \text{Tr}[\rho_\theta T T^\dagger] \\ &= \text{Tr} \left[\rho_\theta \int_{\omega \in \Theta} (\omega - T)(\bar{\omega} - T^\dagger) M(d\omega) \right] \geq 0. \end{aligned}$$

Similarly, (12) is obtained by

$$\begin{aligned} & \int_{\omega \in \Theta} |\omega|^2 \text{Tr}[\rho_\theta M(d\omega)] - \text{Tr}[\rho_\theta T^\dagger T] \\ &= \text{Tr} \left[\rho_\theta \int_{\omega \in \Theta} (\bar{\omega} - T^\dagger)(\omega - T) M(d\omega) \right] \geq 0, \end{aligned}$$

□

Therefore, for the proofs of Theorems 1 and 2, it is sufficient to show that, for the case $\Theta = \mathbb{R}$, if $\text{Tr}[\rho_\theta T] = g(\theta)$ holds for any $\theta \in \Theta$ then

$$\text{Tr}[\rho_\theta (T - g(\theta))^2] = \text{Tr}[\rho_\theta T^2] - g(\theta)^2 \geq {}^t D_k[g(\theta)](J_k^S)^{-1} D_k[g(\theta)],$$

and, for the case $\Theta = \mathbb{C}$, if $\text{Tr}[\rho_\zeta T] = g(\zeta)$ and $\text{Tr}[\rho_\zeta T^\dagger] = g(\bar{\zeta})$ hold for any $\zeta \in \Theta$ then

$$\begin{aligned} & \text{Tr}[\rho_\zeta (T - g(\zeta))(T^\dagger - g(\bar{\zeta}))] \\ &= \text{Tr}[\rho_\zeta T T^\dagger] - |g(\zeta)|^2 \geq D_k^{\mathbb{C}^\dagger}[g(\zeta)](J_k^R)^{-1} D_k^{\mathbb{C}}[g(\bar{\zeta})], \\ & \text{Tr}[\rho_\zeta (T^\dagger - g(\bar{\zeta}))(T - g(\zeta))] \\ &= \text{Tr}[\rho_\zeta T^\dagger T] - |g(\zeta)|^2 \geq D_k^{\mathbb{C}^\dagger}[g(\zeta)](J_k^L)^{-1} D_k^{\mathbb{C}}[g(\bar{\zeta})]. \end{aligned}$$

If $\Theta = \mathbb{R}$, T is a self-adjoint operator, for which the existence of the POVM is trivial. On the other hand, if $\Theta = \mathbb{C}$, one should consider normality and/or subnormality of T with extension of the system. See [6].

Proofs of Theorems 1 and 2.

The Theorem 1 for $\Theta = \mathbb{R}$ and the Theorem 2 for $\Theta = \mathbb{C}$ are proved by using the Schwartz's inequality in a similar way.

If, for any $\theta \in \mathbb{R}$, an self-adjoint operator T satisfies $\text{Tr}[\rho_\theta T] = g(\theta)$, then

$$\begin{aligned}\text{Tr}_{k \times 1}[\rho_\theta L_k^S(T - g(\theta))] &= \text{Tr}_{k \times 1}\left[\frac{\rho_\theta L_k^S + L_k^S \rho_\theta}{2}(T - g(\theta))\right] \\ &= \text{Tr}_{k \times 1}[D_k[\rho_\theta]T] - g(\theta)\text{Tr}_{k \times 1}[D_k[\rho_\theta]] = D_k[g(\theta)].\end{aligned}$$

Let U^S and W^S be column vectors of $k+1$ operators and $k+1$ scalars, respectively, given as

$$U^S := \begin{pmatrix} T - g(\theta) \\ L_k^S \end{pmatrix}, \quad W^S := \begin{pmatrix} 1 \\ -(J_k^S)^{-1}D_k[g(\theta)] \end{pmatrix}.$$

Since

$$\Upsilon^S := \text{Tr}_{k+1 \times k+1}[\rho_\theta U^S (U^S)^\dagger] = \begin{pmatrix} V[T] & {}^t D_k[g(\theta)] \\ D_k[g(\theta)] & J_k^S \end{pmatrix}$$

is non-negative where $V[T] := \text{Tr}[\rho_\theta T^2] - g(\theta)^2$, it holds that

$${}^t W^S (\Upsilon^S)^{-1} W^S = V[T] - {}^t D_k[g(\theta)] (J_k^S)^{-1} D_k[g(\theta)] \geq 0.$$

Hence we obtain the Theorem 1.

If, for any $\zeta \in \mathbb{C}$, an operator T satisfies $\text{Tr}[\rho_\zeta T] = g(\zeta)$, then

$$\begin{aligned}\text{Tr}_K[\rho_\zeta (T - g(\zeta))(L_k^R)^\dagger] &= \text{Tr}_K[(T - g(\zeta))\rho_\zeta (L_k^L)^\dagger] \\ &= \text{Tr}_K[D_k^{\mathbb{C}\dagger}[\rho_\zeta]T] - g(\zeta)\text{Tr}_K[D_k^{\mathbb{C}\dagger}[\rho_\zeta]] = D_k^{\mathbb{C}\dagger}[g(\zeta)]\end{aligned}$$

where $K = k(k+3)/2$. Let U^R and U^L be column vectors of $K+1 = (k+1)(k+2)/2$ operators, and let W^R and W^L be column vectors of $K+1$ scalars, given as

$$\begin{aligned}U^R &:= \begin{pmatrix} T - g(\zeta) \\ L_k^R \end{pmatrix}, \quad U^L := \begin{pmatrix} T - g(\zeta) \\ L_k^L \end{pmatrix}, \\ W^R &:= \begin{pmatrix} 1 \\ -(J_k^R)^{-1}D_k^{\mathbb{C}}[g(\bar{\zeta})] \end{pmatrix}, \quad W^L := \begin{pmatrix} 1 \\ -(J_k^L)^{-1}D_k^{\mathbb{C}}[g(\bar{\zeta})] \end{pmatrix}.\end{aligned}$$

Let $V_1 := \text{Tr}[\rho_\zeta T T^\dagger] - |g(\zeta)|^2$ and $V_2 := \text{Tr}[\rho_\zeta T^\dagger T] - |g(\zeta)|^2$. Since

$$\begin{aligned}\Upsilon^R &:= \text{Tr}_{K+1 \times K+1}[\rho_\zeta U^R (U^R)^\dagger] = \begin{pmatrix} V_1[T] & D_k^{\mathbb{C}\dagger}[g(\zeta)] \\ D_k^{\mathbb{C}}[g(\bar{\zeta})] & J_k^R \end{pmatrix}, \\ \Upsilon^L &:= \text{Tr}_{K+1 \times K+1}[U^L \rho_\zeta (U^L)^\dagger] = \begin{pmatrix} V_2[T] & D_k^{\mathbb{C}\dagger}[g(\zeta)] \\ D_k^{\mathbb{C}}[g(\bar{\zeta})] & J_k^L \end{pmatrix}\end{aligned}$$

are non-negative, it holds that

$$\begin{aligned}(W^R)^\dagger (\Upsilon^R)^{-1} W^R &= V_1[T] - D_k^{\mathbb{C}\dagger}[g(\zeta)] (J_k^R)^{-1} D_k^{\mathbb{C}}[g(\bar{\zeta})] \geq 0 \\ \text{and } (W^L)^\dagger (\Upsilon^L)^{-1} W^L &= V_2[T] - D_k^{\mathbb{C}\dagger}[g(\zeta)] (J_k^L)^{-1} D_k^{\mathbb{C}}[g(\bar{\zeta})] \geq 0.\end{aligned}$$

Hence (8) and (9) of Theorem 2 are satisfied, respectively. \square

B Proofs of Theorems 3 and 4

Lemma 2 If $P(\alpha) := \exp(-\alpha\bar{\alpha}/N)$ for $\alpha \in \mathbb{C}$, then

$$\begin{aligned} & (\alpha - \zeta)^m (\bar{\alpha} - \bar{\zeta})^n P(\alpha - \zeta) |\alpha\rangle \langle \alpha| \\ &= \left(\frac{N}{N+1} \right)^m (a - \zeta)^n (a^\dagger - \bar{\zeta})^m P(\alpha - \zeta) |\alpha\rangle \langle \alpha| \end{aligned} \quad (13)$$

$$= \left(\frac{N}{N+1} \right)^n |\alpha\rangle \langle \alpha| (a - \zeta)^n (a^\dagger - \bar{\zeta})^m P(\alpha - \zeta). \quad (14)$$

Proof. Since $a = \sum_{i=0}^{\infty} \sqrt{i} e_{i-1} e_i^\dagger$ and $|\alpha\rangle = e^{-\alpha\bar{\alpha}/2} \sum_i \alpha^i / \sqrt{i!} e_i$, $a|\alpha\rangle = \alpha|\alpha\rangle$ and $\langle \alpha|a^\dagger = \bar{\alpha}\langle \alpha|$. Moreover, since

$$\begin{aligned} \frac{d}{d\alpha} |\alpha\rangle &= -\frac{\bar{\alpha}}{2} |\alpha\rangle + \exp\left(-\frac{\alpha\bar{\alpha}}{2}\right) \sum_{i=0}^{\infty} \frac{i}{\alpha} \frac{\alpha^i}{\sqrt{i!}} e_i \\ \frac{d}{d\bar{\alpha}} \langle \alpha| &= -\frac{\alpha}{2} \langle \alpha| + \exp\left(-\frac{\alpha\bar{\alpha}}{2}\right) \sum_{i=0}^{\infty} \frac{i}{\bar{\alpha}} \frac{\bar{\alpha}^i}{\sqrt{i!}} e_i^\dagger, \end{aligned}$$

we have

$$\begin{aligned} a^\dagger |\alpha\rangle P(\alpha) &= \exp(-\alpha\bar{\alpha}/2) \sum_{i=0}^{\infty} \frac{i+1}{\alpha} \frac{\alpha^{i+1}}{\sqrt{(i+1)!}} e_{i+1} P(\alpha) \\ &= |\alpha\rangle \left(\bar{\alpha} - \frac{d}{d\alpha} \right) P(\alpha), \end{aligned} \quad (15)$$

$$\begin{aligned} \langle \alpha| a P(\alpha) &= \exp(-\alpha\bar{\alpha}/2) \sum_{i=0}^{\infty} \frac{i+1}{\bar{\alpha}} \frac{\bar{\alpha}^{i+1}}{\sqrt{(i+1)!}} e_{i+1}^\dagger P(\alpha) \\ &= |\alpha\rangle \left(\alpha - \frac{d}{d\bar{\alpha}} \right) P(\alpha) \end{aligned} \quad (16)$$

(for any smooth function $P(\alpha)$), Recursively using these rules (15) and (16) with

$$\frac{d}{d\zeta} P(\alpha - \zeta) = \frac{\bar{\alpha} - \bar{\zeta}}{N} P(\alpha - \zeta) \text{ and } \frac{d}{d\bar{\zeta}} P(\alpha - \zeta) = \frac{\alpha - \zeta}{N} P(\alpha - \zeta).$$

we obtain the results (13) and (14). \square

Lemma 3 Let p and q be non-negative integers and let $n := \frac{(p+q-1)(p+q+2)}{2} + q + 1$. If $p \leq q$, the n -th entry of a Type R operator L_k^R is

$$\begin{aligned} & \sum_{r=0}^{\min(p,q)} (-1)^{\min(p,q)-r} \binom{\max(p,q)}{\min(p,q)-r} \frac{\min(p,q)!}{r!} \\ & \times \frac{(a - \zeta)^{r+\max(0,q-p)} (a^\dagger - \bar{\zeta})^{r+\max(0,p-q)}}{Np(N+1)^{r+\max(0,q-p)}} \end{aligned} \quad (17)$$

The n -th entry of a Type L operator L_k^L is

$$\begin{aligned} & \sum_{r=0}^{\min(p,q)} (-1)^{\min(p,q)-r} \binom{\max(p,q)}{\min(p,q)-r} \frac{\min(p,q)!}{r!} \\ & \times \frac{(a - \zeta)^{r+\max(0,q-p)} (a^\dagger - \bar{\zeta})^{r+\max(0,p-q)}}{Nq(N+1)^{r+\max(0,p-q)}} \end{aligned} \quad (18)$$

Proof. If $p \leq q$, the higher order derivative $(d^{p+q}/d^p\zeta d^q\bar{\zeta})\rho_\zeta$ is calculated as

$$\begin{aligned}
& \frac{1}{\pi N} \int_{\alpha \in \mathbb{C}} |\alpha\rangle \langle \alpha| \frac{d^{p+q}}{d\zeta^p d\bar{\zeta}^q} \exp\left(-\frac{(\alpha - \zeta)(\bar{\alpha} - \bar{\zeta})}{N}\right) d^2\alpha \\
&= \frac{1}{\pi N} \int_{\alpha \in \mathbb{C}} |\alpha\rangle \langle \alpha| \frac{d^p}{d\zeta^p} \left(\frac{\alpha - \zeta}{N}\right)^q \exp\left(-\frac{(\alpha - \zeta)(\bar{\alpha} - \bar{\zeta})}{N}\right) d^2\alpha \\
&= \frac{1}{\pi N} \int_{\alpha \in \mathbb{C}} |\alpha\rangle \langle \alpha| \left(\frac{dz}{d\zeta} \frac{d}{dz}\right)^p \left(\frac{z}{\bar{\alpha} - \bar{\zeta}}\right)^q \exp(-z) d^2\alpha \\
&\quad (z := (\alpha - \zeta)(\bar{\alpha} - \bar{\zeta})/N) \\
&= \frac{1}{\pi N} \int_{\alpha \in \mathbb{C}} |\alpha\rangle \langle \alpha| \frac{(\bar{\alpha} - \bar{\zeta})^{p-q}}{(-N)^p} \exp\left(-\frac{|\alpha - \zeta|^2}{N}\right) \\
&\quad \times \sum_{r=0}^p (-1)^r \binom{q}{p-r} \frac{p!}{r!} \left(\frac{|\alpha - \zeta|^2}{N}\right)^{q-p+r} d^2\alpha.
\end{aligned} \tag{19}$$

Similarly, if $p \geq q$,

$$\begin{aligned}
\frac{d^{p+q}\rho_\zeta}{d^p\zeta d^q\bar{\zeta}} &= \frac{1}{\pi N} \int_{\alpha \in \mathbb{C}} |\alpha\rangle \langle \alpha| \frac{(\alpha - \zeta)^{q-p}}{(-N)^q} \exp\left(-\frac{|\alpha - \zeta|^2}{N}\right) \\
&\quad \times \sum_{r=0}^q (-1)^r \binom{p}{q-r} \frac{q!}{r!} \left(\frac{|\alpha - \zeta|^2}{N}\right)^{p-q+r} d^2\alpha.
\end{aligned} \tag{20}$$

By applying Lemma 2 to (19) and (20), the n -th entry of L_k^R is obtained as

$$\begin{cases} \sum_{r=0}^p (-1)^{p-r} \binom{q}{p-r} \frac{p!}{r!} \frac{(a-\zeta)^{q-p+r} (a^\dagger - \bar{\zeta})^r}{N^p (N+1)^{q-p+r}} & \text{if } p \leq q, \\ \sum_{r=0}^q (-1)^{q-r} \binom{p}{q-r} \frac{q!}{r!} \frac{(a-\zeta)^r (a^\dagger - \bar{\zeta})^{p-q+r}}{N^p (N+1)^r} & \text{if } p \geq q, \end{cases}$$

which means (17). Likewise, the n -th entry of L_k^L is

$$\begin{cases} \sum_{r=0}^p (-1)^{p-r} \binom{q}{p-r} \frac{p!}{r!} \frac{(a-\zeta)^{q-p+r} (a^\dagger - \bar{\zeta})^r}{N^q (N+1)^r} & \text{if } p \leq q, \\ \sum_{r=0}^q (-1)^{q-r} \binom{p}{q-r} \frac{q!}{r!} \frac{(a-\zeta)^r (a^\dagger - \bar{\zeta})^{p-q+r}}{N^q (N+1)^{p-q+r}} & \text{if } p \geq q, \end{cases}$$

which means (18). □

Lemma 4 Suppose that p, q, r, s are non-negative integers and that $p + q$ and $r + s$ are not larger than k . Let

$$m := \frac{(p+q-1)(p+q+2)}{2} + q + 1, \quad n := \frac{(r+s-1)(r+s+2)}{2} + r + 1.$$

Then the (m, n) -th entry of J_k^R is

$$\begin{aligned}
& \frac{d^{p+q+r+s}}{d\kappa^p d\bar{\kappa}^q d\lambda^s d\bar{\lambda}^r} \exp\left(\frac{\kappa\bar{\lambda}}{N} + \frac{\bar{\kappa}\lambda}{N+1}\right) \Big|_{\kappa=\lambda=0} \\
&= \begin{cases} \frac{p!q!}{N^p(N+1)^q} & \text{if } m = n, \\ 0 & \text{if } m \neq n, \end{cases}
\end{aligned} \tag{21}$$

and the (m, n) -th entry of J_k^L is

$$\begin{aligned} & \frac{d^{p+q+r+s}}{d\kappa^p d\bar{\kappa}^q d\lambda^s d\bar{\lambda}^r} \exp\left(\frac{\kappa\bar{\lambda}}{N+1} + \frac{\bar{\kappa}\lambda}{N}\right) \Big|_{\kappa=\lambda=0} \\ &= \begin{cases} \frac{p!q!}{N^q(N+1)^p} & \text{if } m = n, \\ 0 & \text{if } m \neq n. \end{cases} \end{aligned} \quad (22)$$

Proof. Since ρ_ζ is invertible under the assumption $N > 0$, $L_k^R = \rho_\zeta^{-1} D_k^C[\rho_\zeta]$ is a Type R operator for any $\zeta \in \mathbb{C}$. We have

$$\begin{aligned} J_k^R &= \text{Tr}_{K \times K}[\rho_\zeta L_k^R (L_k^R)^\dagger] \\ &= \text{Tr}_{K \times K}[\rho_\zeta^{-1} D_k^C[\rho_\zeta] D_k^{C\dagger}[\rho_\zeta]] \end{aligned}$$

and hence the (m, n) -th entry is

$$\frac{d^{p+q+r+s}}{d\kappa^p d\bar{\kappa}^q d\lambda^s d\bar{\lambda}^r} \text{Tr}[\rho_\zeta^{-1} \rho_{\zeta+\kappa} \rho_{\zeta+\lambda}] \Big|_{\kappa=\lambda=0}. \quad (23)$$

The parameter ζ in (23) can be set to zero because

$$\text{Tr}[\rho_\zeta^{-1} \rho_{\zeta+\kappa} \rho_{\zeta+\lambda}] = \text{Tr}[U \rho_0^{-1} U^{-1} U \rho_\kappa U^{-1} U \rho_\lambda U^{-1}] = \text{Tr}[\rho_0^{-1} \rho_\kappa \rho_\lambda]$$

where $U := \exp(\zeta a^\dagger - \bar{\zeta} a)$. This can be calculated as

$$\begin{aligned} & \text{Tr}[\rho_0^{-1} \rho_\kappa \rho_\lambda] \\ &= \frac{N+1}{(\pi N)^2} \text{Tr} \left[\sum_{n=0}^{\infty} \left(\frac{N+1}{N} \right)^n e_n e_n^\dagger \cdot \int_{\alpha \in \mathbb{C}} |\alpha\rangle \langle \alpha| \exp\left(-\frac{|\alpha - \kappa|^2}{N}\right) d^2 \alpha \right. \\ & \quad \cdot \left. \int_{\beta \in \mathbb{C}} |\beta\rangle \langle \beta| \exp\left(-\frac{|\beta - \lambda|^2}{N}\right) d^2 \beta \right] \\ &= \frac{N+1}{(\pi N)^2} \int_{\alpha \in \mathbb{C}} \int_{\beta \in \mathbb{C}} \exp\left(-\frac{|\alpha - \kappa|^2}{N} - \frac{|\beta - \lambda|^2}{N} + \frac{N+1}{N} \alpha \bar{\beta} \right. \\ & \quad \left. - \alpha \bar{\alpha} - \beta \bar{\beta} + \bar{\alpha} \beta\right) d^2 \alpha d^2 \beta \\ &= \frac{N+1}{(\pi N)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(-{}^t(v - Q^{-1}\mu)Q(v - Q^{-1}\mu) \right. \\ & \quad \left. + \frac{\kappa\bar{\lambda}}{N} + \frac{\bar{\kappa}\lambda}{N+1}\right) dx dy dz dw \end{aligned} \quad (24)$$

where $v := {}^t(x, y, z, w)$, $\mu := {}^t(\text{Re}(\kappa), \text{Im}(\kappa), \text{Re}(\lambda), \text{Im}(\lambda))/N$ and

$$Q := \begin{pmatrix} 1/N + 1 & 0 & -1/(2N) - 1 & -\sqrt{-1}/(2N) \\ 0 & 1/N + 1 & \sqrt{-1}/(2N) & -1/(2N) - 1 \\ -1/(2N) - 1 & \sqrt{-1}/(2N) & 1/N + 1 & 0 \\ -\sqrt{-1}/(2N) & -1/(2N) - 1 & 0 & 1/N + 1 \end{pmatrix}.$$

Since $Q > 0$ and $\det Q = (N+1)^2/N^4$, (24) is equal to

$$\exp\left(\frac{\kappa\bar{\lambda}}{N} + \frac{\bar{\kappa}\lambda}{N+1}\right)$$

so the result (21) is obtained.

Similarly, L_k^L can be given as $L_k^L = D_k^{\mathbb{C}}[\rho_\zeta]\rho_\zeta^{-1}$. Hence

$$J_k^L = \text{Tr}_{K \times K}[L_k^L \rho_\zeta (L_k^L)^\dagger] = \text{Tr}_{K \times K}[D_k^{\mathbb{C}}[\rho_\zeta] \rho_\zeta^{-1} D_k^{\mathbb{C}\dagger}[\rho_\zeta]]$$

so (22) holds. \square

B.1 Proof of Theorem 3

Optimality of (10) for the case $g(\theta) = \theta^2$

First, we formally extend the real parameter θ of ρ_θ to the complex parameter $\zeta = \theta + \sqrt{-1}\eta \in \mathbb{C}$. Then the derivative $(d/d\theta)^k \rho_\theta$ can be considered as $(d/\zeta + d/d\bar{\zeta})^k \rho_\zeta$. A Type S operator $L_2^S = {}^t(L_1, L_2)$ is given as a solution to the equation

$$\frac{d^k}{d\theta^k} \rho_\theta = \left(\frac{d}{d\zeta} + \frac{d}{d\bar{\zeta}} \right)^k \rho_\zeta = \frac{\rho_\theta L_k + L_k \rho_\theta}{2} \quad (25)$$

and $L_k = L_k^\dagger$ for $k = 1, 2$. Let

$$L_k := \sum_{i,j} c_{i,j} (a^i a^{\dagger j} + a^j a^{\dagger i}) \quad (c_{i,j} \in \mathbb{R}).$$

Since each coefficient for $a^i a^{\dagger j}$ in the equation (25) should be zero, the solution is obtained as

$$\begin{aligned} L_1 &= \frac{2}{2N+1} (a + a^\dagger - 2\theta) \\ &= 2 \frac{N+1}{2N+1} \frac{a - \theta}{N+1} + 2 \frac{N}{2N+1} \frac{a^\dagger - \theta}{N} \\ &= 2 \frac{N+1}{2N+1} M_{0,1} + 2 \frac{N}{2N+1} M_{1,0}, \\ L_2 &= \frac{2(a - \theta)^2 + (a^\dagger - \theta)^2}{N^2 + (N+1)^2} + \frac{2(a - \theta)(a^\dagger - \theta)}{N(N+1)} - \frac{2}{N} \\ &= \frac{2(N+1)^2}{N^2 + (N+1)^2} \left(\frac{a - \theta}{N+1} \right)^2 + \frac{2N^2}{N^2 + (N+1)^2} \left(\frac{a^\dagger - \theta}{N} \right)^2 \\ &\quad + 2 \left(\frac{(a - \theta)(a^\dagger - \theta)}{N(N+1)} - \frac{1}{N} \right) \\ &= \frac{2(N+1)^2}{N^2 + (N+1)^2} M_{0,2} + \frac{2N^2}{N^2 + (N+1)^2} M_{2,0} + 2M_{1,1} \end{aligned}$$

where $M_{i,j}$ are Type R operators out of $L_2^R = {}^t(M_{1,0}, M_{0,1}, M_{2,0}, M_{1,1}, M_{0,2})$. As the inner product J_2^R of L_2^R is given in Lemma 4, J_2^S is obtained as

$$J_2^S = \begin{pmatrix} \frac{4}{2N+1} & 0 \\ 0 & \frac{8}{N^2 + (N+1)^2} + \frac{4}{N(N+1)} \end{pmatrix}.$$

Since T of (10) is equal to $(2\theta, 2)(J_2^S)^{-1}L_2^S + \theta^2$, it attains the equality (7), hence it is uniformly optimum. \square

Non-existence of uniformly optimum estimator for the case $g(\theta) = \theta^3$

Since, for all non-negative integers m, n , the leading term of $\text{Tr}[\rho_\theta a^m (a^\dagger)^n]$ is $\theta^m \bar{\theta}^n$, the form of an unbiased estimator for θ^3 of a polynomial form of the creation/annihilation operators is given in the form

$$T = u(a^3 + a^{\dagger 3}) + v(a^{\dagger 2}a + a^\dagger a^2) + w(a^2 + a^{\dagger 2}) + xa^\dagger a + y(a + a^\dagger) + z.$$

Using the characteristic function

$$\begin{aligned} \text{Tr}[\rho_\theta e^{\lambda a^\dagger} e^{\bar{\lambda} a}] &= \frac{1}{\pi N} \int_{\alpha \in \mathbb{C}} \exp\left(\lambda \bar{\alpha} + \bar{\lambda} \alpha - \frac{|\alpha - \theta|^2}{N}\right) d^2 \alpha \\ &= \exp\left((\lambda + \bar{\lambda})\theta + N|\lambda|^2\right), \end{aligned}$$

we have

$$\text{Tr}[\rho_\theta T] = 2\theta^3 u + (2\theta^3 + 4\theta(N+1))v + 2\theta^2 w + (\theta^2 + N+1)x + 2\theta y + z.$$

The unbiasedness condition $\text{Tr}[\rho_\theta T] = \theta^3$ requires that

$$u = \frac{1}{2} - v, \quad w = -\frac{x}{2}, \quad y = -2(N+1)v, \quad z = -(N+1)x.$$

It will be shown that, for any fixed $\theta \in \Theta$, the variance is minimized if

$$\begin{aligned} u &= \frac{N(N+1)}{2(4N^2 + 4N + 3)}, \quad v = 3 \frac{N^2 + N + 1}{2(4N^2 + 4N + 3)}, \\ w &= -\frac{3\theta}{2(2N+1)^2(4N^2 + 4N + 3)}, \quad x = \frac{3\theta}{(2N+1)^2(4N^2 + 4N + 3)}, \\ y &= -3 \frac{(N^2 + N + 1)(N+1)}{4N^2 + 4N + 3}, \quad z = \frac{-3(N+1)\theta}{(2N+1)^2(4N^2 + 4N + 3)}. \end{aligned} \quad (26)$$

Since w, x and z depend on θ , there is no unbiased estimator uniformly minimizing the variance.

By the same way as the previous proof, the third entry of $L_3^S = {}^t(L_1, L_2, L_3)$ can be obtained as

$$\begin{aligned} L_3 &= 2 \frac{(a - \theta)^3 + (a^\dagger - \theta)^3}{N^3 + (N+1)^3} + 6 \frac{(a - \theta)^2(a^\dagger - \theta) + (a - \theta)(a^\dagger - \theta)^2}{N(N+1)(2N+1)} \\ &\quad - 12 \frac{a + a^\dagger - 2\theta}{N(2N+1)} \\ &= \frac{2(N+1)^3}{N^3 + (N+1)^3} \frac{(a - \theta)^3}{(N+1)^3} + \frac{2N^3}{N^3 + (N+1)^3} \frac{(a^\dagger - \theta)^3}{N^3} \\ &\quad + \frac{6(N+1)^2 N}{N(N+1)(2N+1)} \left(\frac{(a - \theta)^2(a^\dagger - \theta)}{(N+1)^2 N} - \frac{2(a - \theta)}{(N+1)N} \right) \\ &\quad + \frac{6(N+1)N^2}{N(N+1)(2N+1)} \left(\frac{(a - \theta)(a^\dagger - \theta)^2}{(N+1)N^2} - \frac{2(a^\dagger - \theta)}{N^2} \right) \\ &= \frac{2(N+1)^3}{N^3 + (N+1)^3} M_{0,3} + \frac{2N^3}{N^3 + (N+1)^3} M_{3,0} \\ &\quad + \frac{6(N+1)^2 N}{N(N+1)(2N+1)} M_{1,2} + \frac{6(N+1)N^2}{N(N+1)(2N+1)} M_{2,1} \end{aligned}$$

where $M_{i,j}$ are Type R operators out of $L_3^R = {}^t(M_{1,0}, \dots, M_{3,0}, M_{2,1}, M_{1,2}, M_{0,3})$. Using Lemma 4, we have

$$J_3^S = \begin{pmatrix} J_2^S & 0 \\ 0 & 0 \end{pmatrix} \frac{24}{N^3 + (N+1)^3} + \frac{72}{N(N+1)(2N+1)}.$$

The unbiased estimator satisfying formulas in (26) is equal to $T = {}^t D_3[\theta^3](J_3^S)^{-1} L_3^S + \theta^3$, which attains the lower bound (8) for the variance at each θ . \square

B.2 Proof of Theorem 4

The holomorphic case $dg/d\bar{\theta} = 0$

Consider the monomial case $g(\theta) = \zeta^k$. The column vector $D_k^{\mathbb{C}}[\bar{\zeta}^k]$ is given as

$$D_k^{\mathbb{C}}[\bar{\zeta}^k] = {}^t \left(0, k\bar{\zeta}^{k-1}, 0, 0, k(k-1)\bar{\zeta}^{k-2}, 0, \dots, 0, \frac{k!}{j!}\bar{\zeta}^j, 0, \dots, 0, k! \right).$$

Lemma 4 shows that J_k^R is a diagonal matrix of the form

$$J_k^R = \text{diag} \left(\frac{1}{N}, \frac{1}{N+1}, \frac{2}{N^2}, \frac{1}{N(N+1)}, \frac{2}{(N+1)^2}, \frac{3!}{N^3}, \dots, \frac{(j-1)!}{N(N+1)^{j-1}}, \frac{j!}{(N+1)^j}, \frac{(j+1)!}{N^{j+1}}, \dots, \frac{(k-1)!}{N(N+1)^{k-1}}, \frac{k!}{(N+1)^k} \right).$$

The system is extended with the ancilla space \mathcal{K} , and the state is set as $\rho_{\zeta} \otimes f_0 f_0^{\dagger}$. The annihilation operator on \mathcal{K} is denoted by b . A Type R operator L_k^R on the extended system is

$$L_k^R = {}^t \left(\frac{a^{\dagger} - \bar{\zeta}}{N}, \frac{a + b^{\dagger} - \zeta}{N+1}, \frac{(a^{\dagger} - \bar{\zeta})^2}{N^2}, \frac{(a + b^{\dagger} - \zeta)(a^{\dagger} - \bar{\zeta})}{N(N+1)}, \frac{(a + b^{\dagger} - \zeta)^2}{(N+1)^2}, \frac{(a^{\dagger} - \bar{\zeta})^3}{N^3}, \dots, \frac{(a + b^{\dagger} - \zeta)^{j-1}(a^{\dagger} - \bar{\zeta})}{N(N+1)^{j-1}}, \frac{(a + b^{\dagger} - \zeta)^j (a^{\dagger} - \bar{\zeta})^{j+1}}{(N+1)^j}, \frac{(a + b^{\dagger} - \zeta)^{k-1}(a^{\dagger} - \bar{\zeta})}{N(N+1)^{k-1}}, \frac{(a + b^{\dagger} - \zeta)^k}{(N+1)^k} \right).$$

Define an operator T_k as

$$T_k := D_k^{\mathbb{C}\dagger}[\zeta^k](J_k^R)^{-1} L_k^R + \zeta^k = \sum_{j=0}^k \binom{k}{j} \zeta^{k-j} (a + b^{\dagger} - \zeta)^j = (a + b^{\dagger})^k.$$

Since $\text{Tr}_{K \times 1}[\rho_{\zeta} L_k^R] = D_k^{\mathbb{C}}[\text{Tr}[\rho_{\zeta}]] = D_k^{\mathbb{C}}[1] = 0$, $\text{Tr}[\rho_{\zeta} T_k] = \zeta^k$. Hence T_k is uniformly optimum unbiased estimator for ζ^k . For the general holomorphic case $g(\zeta) = \sum_k c_k \theta^k$ ($c_k \in \mathbb{C}$), the estimator $T := g(a + b^{\dagger}) = \sum_k c_k T_k$ is unbiased and uniformly optimum. \square

The antiholomorphic case $dg/d\theta = 0$

Consider the monomial case $g(\theta) = \bar{\zeta}^k$. The column vector $D_k^{\mathbb{C}}[\zeta^k]$ is given as

$$D_k^{\mathbb{C}}[\zeta^k] = {}^t \left(k\zeta^{k-1}, 0, k(k-1)\zeta^{k-2}, 0, \dots, 0, \frac{k!}{j!}\zeta^j, 0, \dots, 0 \right).$$

By Lemma 4, J_k^L is a diagonal matrix of the form

$$J_k^L = \text{diag} \left(\frac{1}{N+1}, \frac{1}{N}, \frac{2}{(N+1)^2}, \frac{1}{N(N+1)}, \dots, \frac{(j-1)!}{N^{j-1}}, \frac{j!}{(N+1)^j}, \frac{(j-1)!}{N(N+1)^{j-1}}, \dots, \frac{k!}{N^k} \right).$$

For the annihilation operator b on the ancilla system for the extension $\rho_\zeta \otimes f_0 f_0^\dagger$, a Type L operator L_k^L is

$$L_k^L = {}^t \left(\frac{a^\dagger + b - \bar{\zeta}}{N+1}, \frac{a - \zeta}{N}, \frac{(a^\dagger + b - \bar{\zeta})^2}{(N+1)^2}, \frac{(a - \zeta)(a^\dagger + b - \bar{\zeta})}{N(N+1)}, \dots, \frac{(a - \zeta)^{j-1}}{N^{j-1}}, \frac{(a^\dagger + b - \bar{\zeta})^j}{(N+1)^j}, \frac{(a - \zeta)(a^\dagger + b - \bar{\zeta})^{j-1}}{N(N+1)^{j-1}}, \dots, \frac{(a - \zeta)^{k-1}(a^\dagger + b - \bar{\zeta})}{N^{k-1}(N+1)}, \frac{(a - \zeta)^k}{N^k} \right).$$

Define an operator T_k as

$$T_k := D_k^{\mathbb{C}\dagger}[\bar{\zeta}^k](J_k^L)^{-1}L_k^L + \bar{\zeta}^k = \sum_{j=0}^k \binom{k}{j} \zeta^{k-j} (a^\dagger + b - \bar{\zeta})^j = (a^\dagger + b)^k.$$

Since $\text{Tr}_{K \times 1}[\rho_\zeta L_k^L] = D_k^{\mathbb{C}}[\text{Tr}[\rho_\zeta]] = D_k^{\mathbb{C}}[1] = 0$, $\text{Tr}[\rho_\zeta T_k] = \bar{\zeta}^k$. Hence T_k is uniformly optimum unbiased estimator for $\bar{\zeta}^k$. For the general antiholomorphic case $g(\zeta) = \sum_k c_k \bar{\theta}^k$ ($c_k \in \mathbb{C}$), the estimator $T := g(a^\dagger + b) = \sum_k c_k T_k$ is unbiased and uniformly optimum. \square

The real-valued case $g = \bar{g}$

By Lemmas 3 and 4, $T_{m,n} := D_k^{\mathbb{C}^\dagger}[c_{m,n}\zeta^m\bar{\zeta}^n](J_k^R)^{-1}L_{m+n}^R + \zeta^m\bar{\zeta}^n$ for $k \geq m+n$ is

$$\begin{aligned}
T_{m,n} &= c_{m,n} \sum_{p=0}^n \sum_{q=0}^m \frac{m!n!\zeta^{m-q}\bar{\zeta}^{n-p}}{(m-q)!(n-p)!} \frac{N^p(N+1)^q}{p!q!} \\
&\quad \times \begin{cases} \sum_{r=0}^p (-1)^{p-r} \binom{q}{p-r} \frac{p!}{r!} \frac{(a-\zeta)^{q-p+r}(a^\dagger - \bar{\zeta})^r}{N^p(N+1)^{q-p+r}} & (p \leq q) \\ \sum_{r=0}^q (-1)^{q-r} \binom{p}{q-r} \frac{q!}{r!} \frac{(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p-q+r}}{N^p(N+1)^r} & (p \geq q) \end{cases} \\
&= c_{m,n} \sum_{p=0}^n \sum_{q=0}^m \frac{m!n!\zeta^{m-q}\bar{\zeta}^{n-p}}{(m-q)!(n-p)!} \\
&\quad \times \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r}(a-\zeta)^{q-p+r}(a^\dagger - \bar{\zeta})^r}{(p-r)!(q-p+r)!r!(N+1)^{-p+r}} & (p \leq q) \\ \sum_{r=0}^q \frac{(-1)^{q-r}(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p-q+r}}{(q-r)!(p-q+r)!r!(N+1)^{-q+r}} & (p \geq q). \end{cases}
\end{aligned}$$

$T_{m,n}$ does not depend on $\zeta \in \mathbb{C}$ because $dT_{m,n}/d\zeta$ is equal to

$$\begin{aligned}
& c_{m,n} \sum_{p=0}^n \sum_{q=0}^{m-1} \frac{m!n!\zeta^{m-q-1}\bar{\zeta}^{n-p}}{(m-q-1)!(n-p)!} \\
& \times \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r}(a-\zeta)^{q-p+r}(a^\dagger - \bar{\zeta})^r}{(p-r)!(q-p+r)!r!(N+1)^{-p+r}} & (p \leq q) \\ \sum_{r=0}^q \frac{(-1)^{q-r}(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p-q+r}}{(q-r)!(p-q+r)!r!(N+1)^{-q+r}} & (p > q). \end{cases} \\
& - c_{m,n} \sum_{p=0}^n \sum_{q=1}^m \frac{m!n!\zeta^{m-q}\bar{\zeta}^{n-p}}{(m-q)!(n-p)!} \\
& \times \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r}(a-\zeta)^{q-p+r-1}(a^\dagger - \bar{\zeta})^r}{(p-r)!(q-p+r-1)!r!(N+1)^{-p+r}} & (p < q) \\ \sum_{r=1}^q \frac{(-1)^{q-r}(a-\zeta)^{r-1}(a^\dagger - \bar{\zeta})^{p-q+r}}{(q-r)!(p-q+r)!(r-1)!(N+1)^{-q+r}} & (p \geq q) \end{cases} \\
& = c_{m,n} \sum_{p=0}^n \sum_{q=0}^{m-1} \frac{m!n!\zeta^{m-q-1}\bar{\zeta}^{n-p}}{(m-q-1)!(n-p)!} \\
& \times \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r}(a-\zeta)^{q-p+r}(a^\dagger - \bar{\zeta})^r}{(p-r)!(q-p+r)!r!(N+1)^{-p+r}} & (p \leq q) \\ \sum_{r=0}^q \frac{(-1)^{q-r}(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p-q+r}}{(q-r)!(p-q+r)!r!(N+1)^{-q+r}} & (p > q). \end{cases} \\
& - c_{m,n} \sum_{p=0}^n \sum_{q'=0}^{m-1} \frac{m!n!\zeta^{m-q'-1}\bar{\zeta}^{n-p}}{(m-q'-1)!(n-p)!} \\
& \times \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r}(a-\zeta)^{q'-p+r}(a^\dagger - \bar{\zeta})^r}{(p-r)!(q'-p+r)!r!(N+1)^{-p+r}} & (p \leq q') \\ \sum_{r'=0}^{q'} \frac{(-1)^{q'-r'}(a-\zeta)^{r'}(a^\dagger - \bar{\zeta})^{p-q'+r'}}{(q'-r')!(p-q'+r')!r'!(N+1)^{-q'+r'}} & (p > q') \end{cases} \\
& = 0,
\end{aligned}$$

where $q' := q - 1$ and $r' := r - 1$. $T_{m,n}$ does not depend on $\bar{\zeta}$ because $dT_{m,n}/d\bar{\zeta}$ is equal to

$$\begin{aligned}
& c_{m,n} \sum_{p=0}^{n-1} \sum_{q=0}^m \frac{m!n!\zeta^{m-q}\bar{\zeta}^{n-p-1}}{(m-q)!(n-p-1)!} \\
& \times \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r}(a-\zeta)^{q-p+r}(a^\dagger - \bar{\zeta})^r}{(p-r)!(q-p+r)!r!(N+1)^{-p+r}} & (p < q) \\ \sum_{r=0}^q \frac{(-1)^{q-r}(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p-q+r}}{(q-r)!(p-q+r)!r!(N+1)^{-q+r}} & (p \geq q). \end{cases} \\
& - c_{m,n} \sum_{p=1}^n \sum_{q=0}^m \frac{m!n!\zeta^{m-q}\bar{\zeta}^{n-p}}{(m-q)!(n-p)!} \\
& \times \begin{cases} \sum_{r=1}^p \frac{(-1)^{p-r}(a-\zeta)^{q-p+r}(a^\dagger - \bar{\zeta})^{r-1}}{(p-r)!(q-p+r-1)!(r-1)!(N+1)^{-p+r}} & (p \leq q) \\ \sum_{r=0}^q \frac{(-1)^{q-r}(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p-q+r-1}}{(q-r)!(p-q+r-1)!r!(N+1)^{-q+r}} & (p > q) \end{cases} \\
& = c_{m,n} \sum_{p=0}^{n-1} \sum_{q=0}^m \frac{m!n!\zeta^{m-q}\bar{\zeta}^{n-p-1}}{(m-q)!(n-p-1)!} \\
& \times \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r}(a-\zeta)^{q-p+r}(a^\dagger - \bar{\zeta})^r}{(p-r)!(q-p+r)!r!(N+1)^{-p+r}} & (p < q) \\ \sum_{r=0}^q \frac{(-1)^{q-r}(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p-q+r}}{(q-r)!(p-q+r)!r!(N+1)^{-q+r}} & (p \geq q). \end{cases} \\
& - c_{m,n} \sum_{p'=0}^{n-1} \sum_{q=0}^m \frac{m!n!\zeta^{m-q}\bar{\zeta}^{n-p-1}}{(m-q)!(n-p-1)!} \\
& \times \begin{cases} \sum_{r'=0}^{p'} \frac{(-1)^{p'-r'}(a-\zeta)^{q-p'+r'}(a^\dagger - \bar{\zeta})^{r'}}{(p'-r')!(q-p'+r')!r'!(N+1)^{-p'+r'}} & (p' < q) \\ \sum_{r=0}^q \frac{(-1)^{q-r}(a-\zeta)^r(a^\dagger - \bar{\zeta})^{p'-q+r}}{(q-r)!(p'-q+r)!r!(N+1)^{-q+r}} & (p' \geq q) \end{cases} \\
& = 0,
\end{aligned}$$

where $p' := p - 1$ and $r' := r - 1$. Therefore,

$$\begin{aligned}
T_{m,n} &= c_{m,n} m! n! \begin{cases} \sum_{r=0}^p \frac{(-1)^{p-r} a^{q-p+r} (a^\dagger)^r}{(p-r)! (q-p+r)! r! (N+1)^{-p+r}} & (p \leq q) \\ \sum_{r=0}^q \frac{(-1)^{q-r} a^r (a^\dagger)^{p-q+r}}{(q-r)! (p-q+r)! r! (N+1)^{-q+r}} & (p \geq q) \end{cases} \\
&= c_{m,n} (N+1)^n \sum_{r=0}^{\min(m,n)} (-1)^{\min(m,n)-r} \binom{\max(m,n)}{\min(m,n)-r} \\
&\quad \times \frac{\min(m,n)!}{r!} \left(\frac{a}{N+1} \right)^{r+\max(0,n-m)} a^{\dagger r+\max(0,m-n)}.
\end{aligned}$$

Let $g(\zeta) = \sum_{m,n} c_{m,n}$ be a real-valued polynomial, namely, $c_{m,n} = \overline{c_{n,m}}$. Let $T := \sum_{m,n} c_{m,n} T_{m,n}$. Then, T is a self-adjoint observable. Since $\text{Tr}_{k \times 1}[\rho_\zeta L_k^R] = 0$, $\text{Tr}[\rho_\zeta T_{m,n}] = c_{m,n} \zeta^m \bar{\zeta}^n$. Hence T is an unbiased estimator for $g(\zeta)$. T attains the Type R lower bound because $T = D_k^{\text{C}\dagger}[g(\zeta)](J_k^R)^{-1} L_k^R$.

It can be shown in the same way that $T = D_k^{\text{C}}[g(\zeta)](J_k^L)^{-1} L_k^L$, so that T attains the Type L lower bound too. \square

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